Homework #8, PHY 674, 8 November 1995

Problem X37:

Find the character of the electric dipole operator $\vec{r}$ for the following symmetry groups: O, O_h, T_d, D_{2h}, D_{4h}. Are these characters irreducible ? If not, break them up into irreducible components.

Solution:

Group	O	O_h	T_d	D_{2h}	D_{4h}
$\vec{r}$	Γ_{15}	Γ_{15}	Γ_{15}	$B_{1u} \oplus B_{2u} \oplus B_{3u}$	$A_{2u} \oplus E_u$

Problem X38:

Do the same for the magnetic dipole operator proportional to $\vec{L} = \vec{r} \times \vec{p}$.

Solution:

Group	O	O_h	T_d	D_{2h}	D_{4h}
$\vec{L}$	Γ_{15}	Γ_{15}'	Γ_{25}	$B_{1g} \oplus B_{2g} \oplus B_{3g}$	$A_{2g} \oplus E_g$

Problem X39:

For the groups T_d and D_{2h}, find all allowed electric and magnetic dipole transitions. Which of the phonons (at $\vec{k} = 0$) of $YBa_2Cu_3O_6$ and $YBa_2Cu_3O_7$ are infrared active ?

Solution:

For electric dipole transitions (belonging to the irreducible representation Γ_{15} in T_d), we have to find the characters $\Gamma_i \otimes \Gamma_{15}$ and decompose them. For magnetic dipole transitions, we need to find $\Gamma_i \otimes \Gamma_{25}$. As an example illustrating how to read the table: Electric dipole transitions from a Γ_1 state are allowed to a Γ_{15} state and forbidden to all other states. From a Γ_2 state, only transitions to Γ_{25} are allowed. From a Γ_{15} state, only transitions to Γ_2 are forbidden, all others allowed.

$\Gamma_i(T_d)$	Γ_1	Γ_2	Γ_{12}	Γ_{15}	Γ_{25}
$\Gamma_i \otimes \Gamma_{15}$	Γ_{15}	Γ_{25}	$\Gamma_{15} \oplus \Gamma_{25}$	$\Gamma_1 \oplus \Gamma_{12} \oplus \Gamma_{15} \oplus \Gamma_{25}$	$\Gamma_2 \oplus \Gamma_{12} \oplus \Gamma_{15} \oplus \Gamma_{25}$
$\Gamma_i \otimes \Gamma_{25}$	Γ_{25}	Γ_{15}	$\Gamma_{15} \oplus \Gamma_{25}$	$\Gamma_2 \oplus \Gamma_{12} \oplus \Gamma_{15} \oplus \Gamma_{25}$	$\Gamma_1 \oplus \Gamma_{12} \oplus \Gamma_{15} \oplus \Gamma_{25}$

For D_{2h} (for example the crystal $YBa_2Cu_3O_7$), the electric dipole operator breaks up into the representations $B_{1u} \oplus B_{2u} \oplus B_{3u}$. The magnetic dipole operator breaks up into $B_{1g} \oplus B_{2g} \oplus B_{3g}$. The infrared-active phonons are B_{1u}, B_{2u}, and B_{3u}.

$\Gamma_i(D_{2h})$	A_g	B_{1g}	B_{2g}	B_{3g}	A_u	B_{1u}	B_{2u}	B_{3u}
$B_{1u}\otimes\Gamma_i$	B_{1u}	A_u	B_{3u}	B_{2u}	B_{1g}	A_g	B_{3g}	B_{2g}
$B_{1g}\otimes\Gamma_i$	B_{1g}	A_g	B_{3g}	B_{2u}	B_{1u}	A_u	B_{3u}	B_{2u}
$B_{2u}\otimes\Gamma_i$	B_{2u}	B_{3u}	A_u	B_{1u}	B_{2g}	B_{3g}	A_g	B_{1g}
$B_{2g}\otimes\Gamma_i$	B_{2g}	B_{3g}	A_g	B_{1g}	B_{2u}	B_{3u}	A_u	B_{1u}
$B_{3u}\otimes\Gamma_i$	B_{3u}	B_{2u}	B_{1u}	A_u	B_{3g}	B_{2g}	B_{1g}	A_g
$B_{3g}\otimes\Gamma_i$	B_{3g}	B_{2g}	B_{1g}	A_g	B_{3u}	B_{2u}	B_{1u}	A_u

We also need to do the same for the group D_{4h} in order to study the optical transitions in the $YBa_2Cu_3O_6$ compound. Here, the electric dipole operator breaks up into the irreducible representations $A_{2u}\oplus E_u$. Therefore, the infrared active phonons have the symmetry A_{2u} or E_u. The allowed electric dipole transitions can be found from the following table.

$\Gamma_i(D_{2h})$	A_{1g}	A_{2g}	B_{1g}	B_{2g}	E_g	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_u
$A_{2u}\otimes\Gamma_i$	A_{2u}	A_{1u}	B_{2u}	B_{1u}	E_u	A_{2g}	A_{1g}	B_{2g}	B_{1g}	
$E_u\otimes\Gamma_i$	E_u	E_u	E_u	E_u	$A_{1u}\oplus A_{2u}\oplus B_{1u}\oplus B_{2u}$	E_g	E_g	E_g	E_g	$A_{1g}\oplus A_{2g}\oplus B_{1g}\oplus B_{2g}$

Problem X40:

See the review article by Koster in Solid State Physics, Ref. [25] in the script, particularly the sections starting on page 174 and 229.

Problem X41:

See Koster.

Stefan Zollner, A205 Physics, 294-7327, November 7, 1995.